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Metal-Insulator Transition in a Generalized Hubbard Model

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An extension of the Hubbard model, introduced by Montorsi and Rasetti, is studied using exact diagonalization and quantum Monte Carlo methods. Our numerical results for the static and dynamic properties of one- and two-dimensional systems strongly suggest the occurrence of a metal-insulator transition.

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The correlation effect of electrons has been a subject of interest for many years. A realistic model taking this correlation into account is the Gutzwiller-Hubbard (GH) Hamiltonian [1-5]. In its simplest version, the hopping of the electrons between the Wannier states of neighboring lattice sites leads to a narrow band. Only two electrons of opposite spins occupying the same lattice site interact. The Hamiltonian reads

$$H_{\mathrm{GH}}=-t\sum_{\langle i,j\rangle}\sum_{\sigma}a_{i,\sigma}^{\dagger}a_{j,\sigma}+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}-\mu\sum_{i,\sigma}n_{i,\sigma}\,, \quad (1)$$

where $a_{i,\sigma}^{\dagger}$ and $a_{i,\sigma}$ are the creation and annihilation operators, respectively, for an electron with spin $\sigma=\uparrow,\downarrow$ at lattice site i. $n_{i,\sigma}$ denotes the number operator at site i, and μ the chemical potential. Central problems of interest are, among others, the occurrence of a Mott transition as $|U|$ is increased [6], the magnetic and superconducting nature of the ground state, and the existence of a Fermi surface [7]. In spite of intense efforts [7], the present understanding is still rather limited even in the one-dimensional case where an exact solution has been obtained [6].

Recently, Montorsi and Rasetti (MR) introduced a modified Hubbard model [8,9]. Its Hamiltonian reads

$$H=H_0+H_1\,, \quad (2)$$

$$H_0=U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}-\mu\sum_{i,\sigma}n_{i,\sigma}\,, \quad (3)$$

$$H_1=\tfrac{1}{2}\sum_{\langle i,j\rangle}\sum_{\sigma,\sigma'}t^{\sigma,\sigma'}(a_{i,\sigma}^{\dagger}a_{j,\sigma'}+\mathrm{H.c.})-\tfrac{1}{2}\sum_{\langle i,j\rangle}\sum_{\sigma,\sigma'}\tilde{t}^{\sigma,\sigma'}(a_{i,\sigma}^{\dagger}a_{j,\sigma'}+\mathrm{H.c.})\times(n_{i,-\sigma}+n_{j,-\sigma'}-\gamma n_{i,-\sigma}n_{j,-\sigma'})\,. \quad (4)$$

H differs from the GH model in many respects. It does not conserve the spin. Physically this may be due to the presence of spin-orbit coupling [10]. Moreover, the last term in H_1, describing bond charge repulsion, is reminiscent of the Kivelson-Su-Schrieffer-Heeger (KSSH) model [11]. This term assigns hopping amplitudes which depend on the relative site occupation. Of particular importance is the special case $t^{\sigma,\sigma'}=\tilde{t}^{\sigma,\sigma'}=-t$, where hopping between two singly occupied sites as well as between a doubly occupied and an empty site is inhibited. As a consequence H_0 and H_1 commute, so that the total number of doubly occupied and empty sites is conserved. Note that this is also the case for the original KSSH model, so that this feature is not a consequence of incorporating spin-flip hopping processes. For $\gamma=0$ and 2, the probability for hopping from singly occupied to empty sites and that for hopping from doubly to singly occupied sites are equal.

Assuming a hypercubic lattice and restricting $\sum_{\langle i,j\rangle}$ to nearest neighbors, an exact solution of the model for any number of space dimensions has been proposed, suggesting the occurrence of a metal-insulator transition [8,9]. This transition was often conjectured, but never rigorously established, for a system of interacting electrons. In this Letter we present numerical results as obtained from diagonalization and quantum Monte Carlo (QMC) simulations of finite $d=1$ and $d=2$ systems. Our results strongly suggest that (i) the solution of MR is not exact but provides a good approxiation to the free energy, and that (ii) for $d=1,2$ the model undergoes a metal-insulator transition as a function of U. For this purpose, we calculate the excitation spectrum directly, thereby eliminating the difficult transformation from imaginary to real time [12], the density of states, the momentum distribution of the fermions, the static correlation function for double occupancy, and the free energy.

Following MR [8,9], it is useful to introduce the operators $A_i=(a_{i,\uparrow}+a_{i,\downarrow})/\sqrt{2}$, $N_i=A_i^{\dagger}A_i$, $B_i=(a_{i,\uparrow}-a_{i,\downarrow})/\sqrt{2}$, and $D_i=B_i^{\dagger}B_i$, where D_i commutes with all A_i and $A_i^{\dagger}$. The Hamiltonian then reads

$$H=\sum_{i,j}A_i^{\dagger}M_{i,j}A_j-\mu\sum_{i}D_i\,, \quad (5)$$

where $M_{i,i}=UD_i-\mu$, $M_{i,j}=-t(1-D_i-D_j+\gamma D_iD_j)$ for i,j nearest neighbors, and $M_{i,j}=0$ otherwise. Because $[D_i,H]=0$, the eigenstates of H can be chosen to be simultaneous eigenfunctions of the D_i's and H. The wave function can then be written as $|s_1,\ldots,s_N;n_1,\ldots,n_N\rangle$, where $D_i|s_i\rangle=s_i|s_i\rangle$, $s_i=0,1$, $N_i|n_i\rangle=n_i|n_i\rangle$, $n_i=0,1$, and N denotes the number of lattice sites. In this occupation number representation

$$\langle s_1,\ldots,s_N;n_1',\ldots,n_N'|H|s_1,\ldots,s_N;n_1,\ldots,n_N\rangle=\langle n_1',\ldots,n_N'|H(\{s_i\})|n_1,\ldots,n_N\rangle\,,$$

where $H(\{s_i\})=\sum_{i,j}A_i^{\dagger}M_{i,j}(\{s_i\})A_j-\mu\sum_i s_i$ and $M(\{s_i\})$

is given by $M_{i,j}$ with D_i replaced by s_i. For each set $\{s_i\}$, the tight-binding Hamiltonian $H(\{s_i\})$ describes the hopping of the spinless fermions A_i. Both the hopping amplitudes and local potentials depend on the location ($\{s_i\}$) of the static particles (D_i) [13]. Because $H(\{s_i\})$ is a quadratic form in the A_i's, the trace over the $n_i=0,1$'s can be performed analytically, yielding for the partition function the exact expression

$$Z=\sum_{\{s_i=0,1\}}\det(1+\exp[-\beta M(\{s_i\})])\exp\left(\beta\mu\sum_i s_i\right). \quad (6)$$

In our numerical work we used this exact expression for the partition function. In contrast to the GH model [12], the determinant in (6) is strictly positive. This ensures that there will be no minus-sign problems in the Monte Carlo simulations [12].

One approach to compute (6) and related quantities is to perform the sum over all possible configurations of the $\{s_i\}$. This requires 2^N evaluations of the determinant of the $N\times N$ matrix $1+e^{-\beta M}$. To calculate $e^{-\beta M}$ and the determinant, it is expedient to diagonalize M first, then take the exponent and evaluate the determinant as a product over all eigenvalues. This allows the calculation of the static properties of lattices up to 16 sites with modest computational effort (≈ 2 min on an IBM RISC 6000 M520). For larger systems we use the Metropolis Monte Carlo method to sample the space of the $\{s_i\}$.

To check the free-energy expression derived by MR [8,9], we evaluated this quantity for lattices up to $N=16$ from (6) and according to Eq. (19) of Ref. [8] (see also Ref. [14]). The results listed in Table I clearly reveal that the MR solution is not exact. For a ring of four sites, this can be shown analytically as well. Nevertheless, for the sets of model parameters we have chosen, the MR expression provides a fairly good lower bound for the free energy. The data also illustrate that for $\mu=U/2$ and $\gamma=2$ (corresponding to a half-filled band, i.e., $\rho\equiv N^{-1}\sum_{i,\sigma}\langle a_{i,\sigma}^{\dagger}a_{i,\sigma}\rangle=1$), the free energies for U and $-U$ differ by $|U|/2$, as follows directly from (6).

TABLE I. Free energy per site for a 4×4 lattice, $\beta=\frac{4}{3}$, $\mu=U/2$, $\gamma=2$, $t=1$, and $\rho=1$ with periodic boundary conditions, as obtained from direct numerical evaluation of Eq. (6) (EXACT) and from Eq. (19) of Ref. [8] (MR).

U	EXACT	MR
−12	−0.521	−0.522
−10	−0.524	−0.528
−8	−0.536	−0.548
−6	−0.575	−0.602
−4	−0.681	−0.723
−2	−0.913	−0.963
0	−1.317	−1.370
2	−1.913	−1.963
4	−2.681	−2.723
6	−3.575	−3.602
8	−4.536	−4.548
10	−5.524	−5.528
12	−6.521	−6.522

To explore the occurrence of a metal-insulator transition, we next consider the Fourier-transformed single-particle correlation function

$$G(q,\omega)=\frac{1}{N}\sum_{l,l'}\int_{-\infty}^{+\infty}d\tau\exp[iq(l-l')]\exp[i(\omega-\mu)\tau]\langle\{A_l(\tau),A_{l'}^{\dagger}\}\rangle. \quad (7)$$

From the structure of the partition function (6) it is seen that the time evolution of the integrand is determined by the matrix elements of $e^{i\tau M}$, i.e.,

$$\langle\{A_l(\tau),A_{l'}^{\dagger}\}\rangle=\frac{1}{Z}\sum_{\{s_i=0,1\}}\det(1+\exp[-\beta M(\{s_i\})])\exp\left(\beta\mu\sum_i s_i\right)(\exp[i\tau M(\{s_i\})])_{l,l'}. \quad (8)$$

Because we know the matrix elements of $e^{\tau M}$ for all complex τ numerically, the τ dependence of $\langle\{A_l(\tau),A_{l'}^{\dagger}\}\rangle$ can be evaluated directly. This differs from the usual situation, in which it can be estimated only by continuation from noisy imaginary-time data. In Fig. 1 we depicted $G(q,\omega)$ for a ring of 16 sites at half filling for $U=2$. For fixed q the spectrum consists of two narrow peaks, separated by U. Accordingly the single-particle spectrum of the mobile and spinless fermions (A_i) is nearly exhausted by two well-defined excitation branches. The broadening of the peaks is mainly due to the finite time interval, but the appearance of a broader background is real and must be attributed to an interaction-induced self-energy of the quasiparticles. Additional calculations, not shown here, indicate that both for $d=1$ and $d=2$ and half-filled systems, only one peak occurs for $U=0$, while for $|U|$ that are larger than the ω resolution, two peaks appear at energies $\omega_1(q)=E_q$ and $\omega_2(q)=E_q+U$, where $E_q=-2t\sum_{\nu=1}^{d}\cos q_\nu$. $\omega_1(q)$ and $\omega_2(q)$ correspond to the eigenvalues of $M(\{s_i\})$, where all $s_i=0$ and 1, respectively. The essential features of our numerical results for $G(q,\omega)$ at low temperature are remarkably well described by the approximate expression

$$G_A(q,\omega)=g_q\delta(\omega-\omega_1(q))+(1-g_q)\delta(\omega-\omega_2(q)). \quad (9)$$

Intensity g_q can be related to the exact first frequency moment of $G(q,\omega)$, yielding $g_q=1-\langle D_i\rangle+2E_q(\langle D_i\rangle-\gamma\langle D_iD_{i+1}\rangle)/U$. Equation (9) suggests that with increasing $|U/2dt|$ one reaches a critical coupling above which the two bands no longer overlap and a gap appears. This simple scenario is confirmed by the behavior of the density of states $N(\omega)=N^{-1}\sum_q G(q,\omega)$, a typical exam-

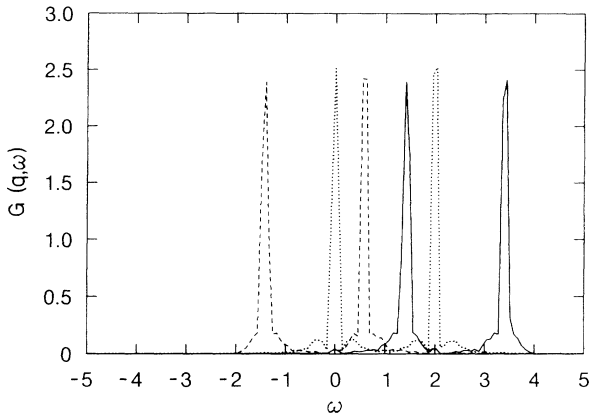

FIG. 1. Spectral function $G(q,\omega)$ for a half-filled ring for $N=16$, $t=1$, $U=2$, $\gamma=2$, $\mu=1$, and $\beta=10$. Solid line, $q=\pi/4$; dotted, $q=\pi/2$; dashed, $q=3\pi/4$.

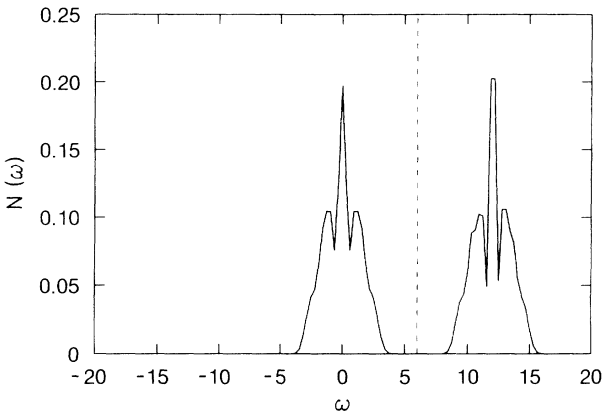

FIG. 2. Density of states $N(\omega)$ for a half-filled 4×4 lattice for $t=1$, $U=12$, $\gamma=2$, $\mu=6$ (dash-dotted), and $\beta=10$.

ple of which is depicted in Fig. 2 for a 4×4 lattice at half filling and $U/2d|t|=3$. Thus, in agreement with (9), the density of states of the half-filled system consists of two bands for $|U/2dt|>2$, each $4d|t|$ wide and separated by $|U|$. Therefore the system is an insulator because the chemical potential $\mu=U/2$ is located within the gap, while for $|U/2dt|<2$ the two bands overlap and μ separates occupied and unoccupied states, a characteristic of the metallic state.

To substantiate the metal-insulator transition scenario further, we have also calculated the momentum distribution of the fermions $n_q=\langle a_{q,\uparrow}^{\dagger}a_{q,\uparrow}\rangle+\langle a_{q,\downarrow}^{\dagger}a_{q,\downarrow}\rangle=\langle A_q^{\dagger}A_q\rangle+N^{-1}\sum_i\langle D_i\rangle$. The numerical results are depicted in Fig. 3, where we subtracted $N^{-1}\sum_i\langle D_i\rangle$, the contribution of the immobile particles. For comparison we included $N_q=n_q-N^{-1}\sum_i\langle D_i\rangle$ calculated from (9), leading to a sum of two Fermi distributions. For $U=0$, N_q is seen to follow rather closely the Fermi distribution even though the Hamiltonian H does not reduce to a free-fermion Hamiltonian for $U=0$. In the metallic regime ($|U/2dt|<2$), there are two overlapping bands. Here one expects according to (9) two Fermi wave vectors q_F where N_q drops abruptly, exhibiting a plateau in between. For $d=1$, $U=-2|t|$, and $N^{-1}\sum_q N_q=\frac{1}{2}$, we have $q_F=\pi/3$ and $q_F=2\pi/3$. In the insulating phase, however, the lower band is filled and N_q remains constant. These features resulting from the simple band picture and the assumption of well-defined quasiparticles are in remarkable agreement with the numerical results shown in Fig. 3.

For $\rho\neq 1$ our numerical results (not shown) for $d=1,2$ indicate the following: For $U<-4d|t|$, there is a line $U_c=U_c(\rho)$ where the system undergoes a metal-insulator transition. In the metallic phase $U>U_c$ there is another line $U^*=U^*(\rho)$, where $G(q,\omega)$ exhibits one (for $U>U^*$) or two (for $U<U^*$) peaks for fixed q. This behavior is again well described by the approximate expression (9), leading to $\rho=2\langle D_i\rangle$ for the equation determining U_c. U^* is given by the minimum value of U where both $\langle D_i\rangle$ and $\langle D_iD_{i+1}\rangle$ vanish.

Finally, we consider the expectation value for double occupancy $V=V(U)\equiv\langle n_{i,\uparrow}n_{i,\downarrow}\rangle=-\beta^{-1}\partial\ln Z/\partial U$. Accordingly, a metal-insulator transition at $T=0$ driven by U will be signaled by discontinuous behavior at $U=U_c$. This is confirmed by our numerical results. For $T\to 0$ and $|U/2dt|>2$, V tends to a constant value: 0 for $U>0$ and $\frac{1}{2}$ for $U<0$; while in the metallic phase V decreases with U. The symmetry mentioned above implies that $V(-U)+V(U)=\frac{1}{2}$ for $\rho=1$, $\gamma=2$, and $U=2\mu$. For $|U|\to\infty$ the system becomes classical so that at $T=0$, $V\to 0$ due to strong repulsion, while in the attractive case

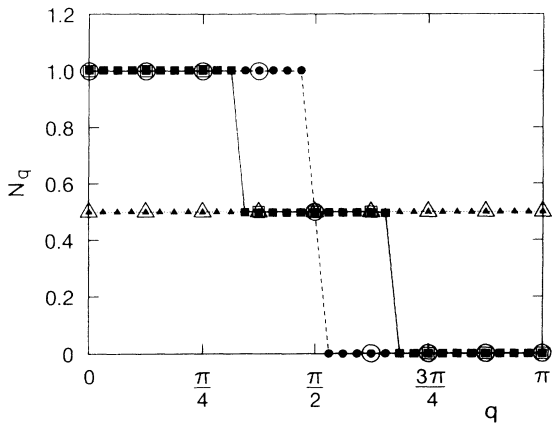

FIG. 3. Occupation number N_q for half-filled rings for several U and $\beta=100$. Solid line, calculated using $G_A(q,\omega)$ for $U=2|t|$; dashed, calculated using $G_A(q,\omega)$ for $U=0$; dotted, calculated using $G_A(q,\omega)$ for $U=6|t|$. ●, QMC data for a ring of 64 sites and $U=0$; ○, exact results for a ring of 16 sites and $U=0$. ■, QMC data for a ring of 64 sites and $U=2|t|$. □, exact results for a ring of 16 sites and $U=2|t|$; ▲, QMC data for a ring of 64 sites and $U=6|t|$; △, exact results for a ring of 16 sites and $U=6|t|$.

$V \to \frac{1}{2}$.

In summary, we have shown that the solution [8] of the MR model is not exact. Our numerical results demonstrate that the system is particularly interesting in that it exhibits a metal-insulator transition and its real-time dynamic properties are amenable to an accurate numerical treatment.

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[14] We thank A. Montorsi and M. Rasetti for pointing out a misprint in their Eq. (19).